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A FACILITY FOR LARGE-SCALE HAZARDOUS GAS TESTING INCLUDING RECENT TEST RESULTS

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INTRODUCTION

The U.S. Department of Energy (DOE) is in the process of constructing a spill test facility for liquefied gaseous fuels and other hazardous materials in the Frenchman Flat basin on the Nevada Test Site (NTS) as shown in Fig. 1. The Lawrence Livermore National Laboratory (LLNL) is assisting DOE in construction of that facility and will be assisting with facility operation when construction is complete in January, 1986.

The facility is designed 1) to discharge, at a controlled rate, a known amount of hazardous test fluid onto the surface of the dry lake bed; 2) to monitor and record process operating data, meteorological data, downwind gas concentration data, and other data as is required for the experiment; and 3) to provide a means to control and monitor these functions from a remote location. This design is described in detail by Johnson and Thompson, 1984.

The spill facility consists of two generally separate process systems. The larger and more complex of the two is designed to handle cryogenic fluids such as LNG. The noncryogenic spill system is designed to handle fluids which are normally stored and shipped as pressurized liquids, such as ammonia.

The NTS and the surrounding Nellis Air Force Range is remote and not open to public access. The area downwind of the spill facility is essentially unpopulated with access strictly controlled all the way to the Nellis boundary, 60 km (40 mi) away. This will allow testing with hazardous and toxic substances which could not be done anyplace else in the U.S.

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Large-scale spill tests of ammonia and nitrogen tetroxide were performed at NTS in 1983 using a portable facility. Results from these tests are just now being made publicly available and are presented here, in preliminary form, as an example of what can be accomplished at the new facility.

FACILITY PERFORMANCE CRITERIA

Many potential facility users have expressed needs for information to aid them with risk assessment, emergency response, regulation, plant design, and plant siting. Researchers working in the related fields of dense gas dispersion, vapor cloud combustion, and other scientific disciplines central to understanding accidents associated with the transportation and storage of hazardous substances, have suggested a number of capabilities the facility should have. It should be capable of source definition experiments on a variety of spill surfaces. Perhaps the most important need is for model validation experiments for both theoretical and wind tunnel models. These models must eventually be relied upon for hazard prediction, since it is not possible to test all potential accident scenarios. Tests would involve measuring gas dispersion distances for a substance for a variety of atmospheric conditions. Once the extent of the problem is determined, the next priority is the development and evaluation of mitigation techniques and equipment. Examples of such techniques currently being evaluated as means for mitigating the effects of dense gas releases are water-spray curtains and vapor fences. In addition, the blast and flame hazards associated with flammable material under varying plant and accident situations are of interest to many. The effects of terrain, buildings, and obstructions are of general concern because they can be extremely important and highly individualized.

The facility is designed to test materials from each of the generic categories: cryogenic, aerosol forming, chemically reactive, isothermal (high pressure), and with some minor modifications, superheated liquids. The tests are designed to reproduce accidental releases as closely as possible, using the actual materials of concern.

Performance criteria appropriate for the two general categories of test fluids are given in Table I. All fluid parameters given are in liquid phase and, except for noncryogenic spill rate, represent the total capacities of the process systems. Depending on the toxicity of the test fluids, environmental constraints might require that the maximum spill volumes be reduced to some level below these capacities. Such tests will be scaled down to some level as part of the operational requirements in order to accommodate applicable environmental constraints. The facility is designed specifically for the fluids listed in Table I, however, it will accommodate other materials which have similar and compatible physical properties. The process flow diagram for the facility is shown in Fig. 2, and an overhead view of the facility under construction is shown in Fig. 3.

TABLE I. SPILL FACILITY PERFORMANCE CRITERIA

Materials	Temp (°C)	Vapor Pres. (pa)	Density (kg/m^3)	Spill Volume	Spill Rate
CRYOGENIC SYSTEM					
LNG	-162	9.1×10^4	447	Minimum 5 m^3 (1320 gal); Maximum 200 m^3 (52,800 gal)	Minimum 5 m^3/min (1320 gpm); Maximum 100 m^3/min (26,400 gpm)
LPG	-44	9.1×10^4	581		
NH_3	-36	9.1×10^4	679		
Ethylene	-106	9.1×10^4	570		
NONCRYOGENIC SYSTEM					
Cl_2	38	1.07×10^6	1352	Minimum 3 m^3 (792 gal); Maximum 90 m^3 (23,775 gal)	Minimum 2 m^3/min (528 gpm); Maximum 20 m^3/min (5,280 gpm)
N_2O_4	38	2.14×10^5	1402		
LPG	38	1.29×10^6	481		
NH_3	38	1.46×10^6	583		
Cyclohexane	38	2.27×10^4	759		
Hydrazine	38	$< 7 \times 10^3$	992		

FACILITY DESIGN

The performance requirements in the above section have been used to develop the Facility configuration discussed here.

NITROGEN STORAGE AND SUPPLY SYSTEM

The nitrogen storage and supply system will provide drive, cooldown, and purge gas to the facility. This system is shown schematically in Fig. 2. This system provides nitrogen gas at controlled pressures varying from 120 to 280 psig (8.3×10^5 to 1.9×10^6 pa) to force test fluid out of the storage tanks and through the spill pipe(s) to the spill point. Nitrogen is also provided for purging tanks and piping prior to their use, and for remote-controlled valve actuation. Each of the two storage tanks has a design pressure of 2500 psig (1.72×10^7 pa) and a volume of 2366 ft^3 (67-m^3).

Drive gas is routed to the upstream end of the spill pipes to drive out residual quantities of test fluid during the late stages of a test and to drive fluid from the spill pipe(s) if small quantities of fluid are being spilled. This procedure involves isolating and bypassing the storage tanks.

The source of nitrogen gas will be a liquid nitrogen (low pressure) storage tank with a high pressure cryogenic discharge pump providing pressurization into the 2000 psi (1.38×10^7 pa) tanks. The vaporizer is an atmospherically heated unit.

Liquid nitrogen or cold nitrogen gas will be used to precool the cryogenic piping and tankage prior to introduction of fluids into these systems. Precooling will be done by introducing nitrogen liquid or gas at near -310°F (-190°C) into the system and venting it out the downstream ends of the systems. The precool system will consist of liquid nitrogen provided in the LN_2 storage tank, a low-pressure nitrogen vaporizer, a temperature control system on the vaporizer outlet and pipe connections to the cryogenic spill system. Temperature monitoring of piping and tanks is used to control the flow of cold fluid or gas into these sections during cooldown.

CRYOGENIC SPILL SYSTEM

The cryogenic spill system, also shown in Fig. 2, consists of means for receiving and storing cryogenic fluids and for discharge of the fluids at the spill point.

The cryogenic storage system receives test fluids delivered by tanker truck and provides storage during periods of test operations. The system consists of two (2) tanks, valves, vent piping, transfer piping and process instrumentation (level, pressure, temperature, and flow).

The two cryogenic tanks each have capacities of 100 m^3 (26,000 gal). The cryogenic storage tanks are provided with valves and piping used for unloading test fluid into the storage tanks and transferring fluid from one tank to another. Vent and pressure-relief valves are provided. Boil-off is controlled through a back-pressure control valve. Vent piping leads from the cryogenic tanks and piping to a vent stack. The tanks are instrumented with vacuum and pressure gauges, thermocouples and liquid-level sensors.

The two cryogenic storage tanks are each connected separately to 500-ft (152 m) long spill piping. Tank C-105 is connected to two (2) separate lines; a 12-in (0.3 m) line to provide high-flow capability, and a 6-in (0.15 m) line to handle the lower flow rate tests. The second cryogenic tank, C-106, is connected to a single 12-in (0.3 m) line. Each spill pipe is equipped with control valves at each end. Restrictive orifices at the downstream ends are provided to develop adequate back pressure along the line to prevent flashing within the pipe during the spill.

The upstream end of each spill pipe is ground-anchored; the downstream end is allowed to move to accommodate thermal expansion. The piping is also provided with relief valves which discharge into the vent system.

NONCRYOGENIC FLUID SPILL SYSTEM

To accommodate those test fluids which are not stored in cryogenic facilities, an auxiliary noncryogenic fluid system is provided. This system is also shown schematically in Fig. 2. The storage tank used for this purpose, a 24,000 gal. (90 m^3) tank of carbon steel construction, is designed for a working pressure of 300 psig (2.1×10^6 pa). The tank is instrumented with pressure gauges, thermocouples and liquid level sensors. Pressure relief is into the vent system.

This tank is connected through valving and piping to all three (3) spill pipes. (The spill lines are used interchangeably for both cryogenic and noncryogenic fluids) Spool sections which are removable are used to make intermittent connection to the spill lines. These disconnects are provided to eliminate stresses in the close-coupled piping caused by thermal cycling of the lines when in cryogenic use.

VENT SYSTEM

The vent system consists of a gathering header and a 400-ft (122 m) long transport header which discharge into the base of a 40-ft (12 m) high vent stack. The vent stack is located downwind from the storage tank area. This system is designed and sized to transport vented gases from any of the test fluids systems at those maximum flow rates anticipated during off-normal conditions. Routine venting, such as during fluid transfer into the spill pipe(s), will also be done through this system.

COMMAND, CONTROL AND DATA ACQUISITION SYSTEM (CCDAS)

The Command, Control and Data Acquisition System (CCDAS) serves as the overall control center for the Spill Facility including the data acquisition system. The objectives of this system are:

a) To provide remote and local control for the process system.

b) To monitor important parameters and status information within the process system.

c) To provide for control of, and recording of data from, the LGF Data Acquisition System (up to 61 remote stations) and the new high-speed data acquisition subsystem.

The system consists of modern industrial control computer hardware and software of proven reliability and performance, plus the LGF Data Acquisition System (Baker, 1982).

Process Control Subsystem. At the spill site a local subsystem (microcomputer-based) provides signal conditioning for both input and output, provides local monitoring and control for manual operation and check-out purposes and supports communications with the CCDAS building. At the CCDAS building, located approximately one mile to the west, is the operator's console and main computer hardware. Through a high speed data link, the operators are able to observe and control the various functions of the spill procedure, as well as acquire diagnostic data from the downwind sensor array, all in real time.

In order to prevent accidental fluid releases, personal injury, or equipment damage, all elements are designed using fail-safe criteria, some of which are listed as follows:

a) Remote location of the control center so that, in emergencies, all critical valves can be safely closed by operating personnel.

b) Automatic shutdown if a critical out-of-range condition is detected, as would be the case if a pressure regulator failed.

c) The pneumatically-operated valves return to their safe (closed) position by spring action if instrument gas (N_2) pressure is lost. In addition, the solenoid valves and current-to-pressure converters close in a loss-of-power condition, thus closing the control valve.

d) If communications should be lost between the remote and local computers, the local system is programmed to automatically return the entire facility to a safe state.

e) As a manual backup to computer-facilitated communications, critical valves, such as the spill valves, will be connected directly by wire to the remote operator's console as an emergency shutoff.

f) All electronic control elements, including the computer, will have built-in initialization hardware such that all outputs come up safe at power-on.

Interlocks, both mechanical and electrical, are an integral part of the control subsystem. The operator's console contains keyinterlock switches and software checks to prevent inadvertent or inappropriate valve actuations. In the field the local control computer is similarly equipped so that remote operations cannot be performed until the equipment is electrically "armed" via an interlock switch. In addition, there are various ways of mechanically locking off valves such that remote operation is physically impossible.

High Speed Data Acquisition Subsystem. In order to satisfy the need for intensive high-speed measurements of physical quantities near the spill point, special analog and digital inputs are allocated. These inputs would be assigned to special instruments prior to each test for permanent data recording. Typical of these are fast anemometers for turbulence analysis, on-line gas detectors, radiometers, and blast gauges for combustion tests. Digitizing rates of over 1000 samples/second per channel are available. This system shares the resources of the process control and monitoring computer.

Liquefied Gaseous Fuels Data Acquisition System (LGFDAS). The LGFDAS is designed as a general-purpose, portable data acquisition system for use in spill tests. This system consists of an array of 61 remote monitoring stations. This array is made up of 20 anemometer stations to gather wind speed and wind direction data, 41 sensor stations to gather data from a large variety of sensors at various levels above ground, a meteorological tower, and photographic stations. The sensors deployed at the sensor stations will include several hundred instruments to measure gas concentration (including IR absorption), humidity, heat flux, aerosol characteristics, turbulence (sonic and bivane anemometers), and flame speed. The sensor array and the associated data acquisition system is battery powered and will be linked to the control point by means of telemetry. This system is not directly connected with the operation of the spill facility and is used for the bulk of the downwind physical measurements made during a spill test. In addition, it provides realtime micrometeorological monitoring in the vicinity of the spill site which is used in determining wind conditions for a test. The LGFDAS computers and displays are located in the CCDAS building with the process control and monitoring equipment for operator convenience. A detailed description of the LGFDAS is included in Baker 1982.

TEST CAPABILITIES

DESIGN BASIS

The facility has been designed to have the capabilities necessary to meet the testing needs of its potential users. Among those needs expressed are that the facility provide information complementary to that produced by the

Thorney Island Trials (Health and Safety Executive, 1983). A graphical review of these tests and others, including our recent Desert Tortoise and Eagle Series, and showing the range of applicability of the new facility, is given in Fig. 4. To that end, the facility has been designed to reproduce the size and rate of accidental releases as closely as possible with the actual materials of concern. Thus, the effects of cryogenic temperatures and aerosols on dispersion can be observed directly. This makes the facility ideally suited for the validation of models, both theoretical and wind tunnel, for the observation and measurement of new and/or important phenomena, and for the design and evaluation of protective measures such as water curtains and vapor barriers. In its current, basic configuration, the facility can accommodate dispersion tests and combustion tests, such as pool fires (on soil) and vapor cloud fires with only a minimal amount of additional thermal shielding of sensitive components near the end of the spill pipes.

WATER SURFACE CONFIGURATION

A modification to the basic configuration will be required to accommodate those tests of LGF's, such as dispersion and pool fires (on water) and rapid phase transitions, which require the discharge of test fluids on water. This modification, may require temporary extension of the spill pipe(s) on temporary supports to a point a safe distance away from the design basis spill point. A pond will need to be constructed about this point to provide the water surface. This is easily done since the surface of Frenchman Flat is mostly clay and nearly impervious to water and water will be available at the tank farm.

RAPID RELEASE CONFIGURATION

A modification to the basic configuration will be required to accommodate those tests of LGF's which, by their nature, require an extremely rapid or explosive release of test fluids into the atmosphere. The creation of fireballs and Boiling Liquid Expanding Vapor Explosions (BLEVE) are examples of this type of testing. This release could be created from a pressurized tank positioned downwind from the spill point. The location would be at a safe distance from the spill pipes and facility components such that no damage would be sustained by the facility.

REVIEW OF RECENT TESTING

As an example of the type of testing planned for the new facility, and the testing conditions available at NTS, two recent test series will be reviewed. A series of large-scale (15-60 m^3) NH_3 spill tests was conducted for the U.S. Coast Guard, The Fertilizer Institute, and Environment Canada; and a series of large-scale (3-5 m^3) N_2O_4 spill tests was conducted for the U.S. Air Force by LLNL during the summer/fall of 1983 (McRae, et al., May 1984, June 1984, March 1985; Goldwire, August 1985; Goldwire, et al., in preparation). The NH_3 tests, called the Desert Tortoise series, and the N_2O_4 tests, called the Eagle series, were conducted using a temporary spill facility on the Frenchman Flat area of NTS at essentially the same location at which the new DOE facility is currently being built. The major purpose of both test series was to measure the atmospheric dispersion of the spilled material for simulated accidental releases under various meteorological conditions. The N_2O_4 tests had the additional goals of providing source strength measurements under varying wind conditions and of providing an opportunity to test foam vapor suppression equipment and emergency response procedures.

DATA ACQUISITION SYSTEM

The measurement and data acquisition system used for these tests is part of the system which will be available for testing at the new facility. Measurements of temperature, flowrate, and heat flux were made at the spill point. In addition to the spill area measurements, atmospheric boundary layer, wind field, vapor cloud temperature and concentration, and surface heat flux measurements were also made using this diagnostic system. There were three main arrays of diagnostic instruments: the meteorological array, the mass flux array, and the dispersion array. The locations of the various stations making up these arrays, along with the positions of the camera stations, are shown in Fig. 5.

The meteorological array for these tests consisted of eleven two-axis, cup-and-vane anemometers (all at a height of 2 m), plus a 20-m tall met. tower located directly upwind of the spill area. The locations of the anemometer stations are shown in Fig. 5. Wind speed and direction at each station were averaged for 10 sec, and the results, plus the standard deviation of direction for the same period, were transmitted back to the Command Control and Data Recording trailer and displayed in real time. This display was the primary information used to determine the optimum time for the spill.

The meteorological tower was outfitted with four temperature gauges and three Gill bivane anemometers. This station also measured the ground heat flux. Humidity data and local barometric pressure were obtained from the NTS Weather Support Group.

A mass flux array was employed to determine the evaporation rate, or source strength. This was accomplished by measuring the gas/ aerosol concentration, vapor cloud temperature and velocity as it passed through the array. The product of the mass density and velocity integrated over the vapor cloud cross-section yields the total mass flux passing through the array at any instant. If the entire cloud is within the array, this mass flux should be equivalent to the source strength of the spilled material.

The mass flux array was located 100 m downwind of the spill area for the NH_3 tests and 25 m for the N_2O_4 tests. It consisted of seven gas stations and two anemometer stations. The centerline station was a 10 m tall tower outfitted with three bivane anemometers, plus gas, temperature, aerosol, and heat flux sensors. The remaining six stations had 6 m tall masts and each was outfitted with gas and temperature sensors, with the stations located at 5-m intervals to either side of the centerline station (three to each side). For the NH_3 tests, vapor concentrations were measured using MSA nondispersive IR gas sensors at 1, 3, and 6 m heights. Gas plus aerosol was passed through a heating apparatus to vaporize the aerosol and allow the total amount of NH_3 present to be determined.

A detailed description of the LLNL IR gas sensor is given in Bingham et al. (1983). The sensor produces a signal proportional to the molecular absorption of IR radiation by the N_2O_4 or NH_3 vapors as they pass through the 15 cm sample region. The sensor was calibrated by using known concentrations of N_2O_4 or NH_3.

The dispersion array consisted of five 10 m towers located approximately 800 m downwind of the spill area (see Fig. 5). The purpose of this array of sensors was to measure the downwind dispersion by recording the concentration and dimensions of the gas cloud during each spill test. All the towers had gas sensors and thermocouples located at heights of 1, 3.5, and 8.5 m above the ground. A typical data acquisition station of this type is shown in Fig. 6. The towers were separated by a distance of 100 m. In addition, there were portable ground-level stations at 2800 m, and on occasion, at 5500 m downwind.

The control of the spills and the data acquisition and storage was all performed in the CCDRS trailer. This system utilizes UHF radio telemetry for command and data transmission and is designed to acquire data from sensors distributed over an area with a diameter of up to 10 miles (Baker, 1982). All of the remote data acquisition stations and sensors are battery-powered, portable, gas-tight, and ruggedized. Batteries are recharged by solar cells. This network of 24 stations acquired data from up to 285 channels at a rate of one sample per second for the gas and control stations and one sample per 10 seconds for the wind-field stations.

After each test, raw data are converted to calibrated data sets. These reduced data are written to an ASCII magnetic tape and transferred to the LLNL Computation Center for verification and archival preservation. The data base tables are stored on an off-line mass storage system and are readily available for analysis.

RESULTS

The extensive instrumentation on the recent large-scale spill tests of ammonia (NH_3) and nitrogen tetroxide (N_2O_4) has resulted in a large amount of data which can be used to quantitatively describe the observed phenomena. Test summaries, listing spill conditions and meteorological conditions, are given in Table II and III for the two test series. Estimates of stability class came from vertical termperature gradients and horizontal wind variability σ_θ.

TABLE II. TEST SUMMARY FOR DESERT TORTOISE SERIES NH_3 SPILLS.

Test	Date	Size (m^3*)	Rate (m^3/min)	Wind speed (m/s)	Wind direction	Stabilty class
1	8/24	15	7.0	7.4	224°	D
2	8/29	44	10.3	5.7	226°	D
3	9/1	32	11.7	7.4	219°	D
4	9/6	60	9.5	4.5	229°	E

* 1 m^3 = 264 gallons

TABLE III. TEST SUMMARY FOR EAGLE SERIES N_2O_4 SPILLS.

Test	Date	Size (m^3*)	Rate (m^3/min)	Wind speed (m/s)	Wind direction	Stabilty class
1	9/17	1.3	1.75	6.2	233°	C
2	9/23	1.5	1.4	5.8	223°	A
3	10/7	4.2	1.4	3.1	229°	D
4	10/13	2.8	0.5	4.9	233°	D
5	10/16	1.3	0.6	2.2	261°	A
6	10/30	3.4	0.7	5.0	223°	D

* 1 m^3 = 264 gallons

Selected results will be presented here with the intention that they serve merely as examples of data which could be obtained at the facility. Other publications will present the results more completely (McRae et al., May 1984, June 1984, March 1985; Koopman et al., Nov. 1984; Goldwire, August 1985; Goldwire, to be published).

N_2O_4 RESULTS

The Eagle 3 and Eagle 6 tests involved N_2O_4 spilled unconfined onto the desert soil from the multiple-exit configuration. They were conducted under nearly ideal atmospheric conditions for the observation of dense gas effects on dispersion, one of the goals of the test series. The vapor cloud traveled directly down the array centerline producing NO_2 concentrations in excess of 500 ppm for Eagle 3 and 315 ppm for Eagle 6 at 785 m. One of the portable NO_2 sensors located on the array centerline at 2800 m recorded a peak concentration of 9 ppm for Eagle 3.

As the liquid N_2O_4 spilled, it was observed to evaporatively cool to its freezing point. The ground heat flux as measured directly below the soil surface in the spill area is shown in Fig. 7 for Eagle 3. The sign convention for the ground heat flux is such that a positive value represents heat flowing <u>into</u> the ground. The change in heat flux during the spill was much less than expected. Assuming that the multi-exit spill system distributed the N_2O_4 uniformly over a 20 m diameter area, and that it evaporated as fast as it was spilled, would require a total heat flux of about 50 kWatt/m^2. We see from Fig. 7 that the peak measured ground heat flux is about 100 times less than this amount. Thus, heat transfer from the ground accounts for the vaporization of only about 23 kg/min of the spilled N_2O_4. Since the spill rate was about 2030 kg/min, clearly the N_2O_4 did not evaporate as quickly as it was spilled. Similar results hold for Eagle 6.

It became apparent upon examination of the Eagle 1 spill results that something other than N_2O_4 and/or NO_2 vapors was present in the vapor cloud. The LLNL IR sensor detects molecular absorption in four different spectral regions. For mixtures of N_2O_4 and NO_2 vapors, two spectral regions experienced absorption (signal channels) while the other two did not (reference channels). If only N_2O_4 or NO_2 vapors were to pass through the sensor absorption region, strong attenuation would be expected in the signal channels and little attenuation would be expected in the reference channels. For all of the Eagle series spills the observed attenuation in the reference channels was almost equivalent to that of the signal channels.

Prior to the Eagle 3 spill, the IR sensors were tested using N_2O_4 vapors directly from the tanker. The sensors behaved as expected, showing little attenuation in the reference channels. During the Eagle 3 spills, grab samples of the vapors were obtained as the cloud passed through the 25 m array. A grab sample of the vapors of the N_2O_4 in the spill pipe was also obtained. These grab samples were analyzed later at LLNL by both mass and IR spectroscopy. None of the grab sample results indicated the presence of a foreign gas capable of producing the broad-band (4-channel) attenuation observed in the Eagle series tests. It was concluded that the attenuation must be due to aerosol scattering which does produce broad-band attenuation. Furthermore, the photography of the spills shows what appears to be a definite two-phase region within the vapor cloud.

The source of the aerosol is believed to be a result of the gas-phase reaction of NO_2 with the ambient humidity, i.e.,

$$3\ NO_2 + H_2O \rightarrow 2\ HNO_3 + NO$$

This reaction, and the resulting HNO_3 mist formation, has been studied in regard to scrubbing NO_2 from exhaust stacks (Goyer, 1963; England, 1974; Peters, 1955; Chambers, 1937; McRae, May 1984). The reaction is extremely fast. Experiments have shown that for typical atmospheric humidities and NO_2 concentrations greater than 50 ppm, a HNO_3 mist is instantly formed. An HNO_3 mist would also explain the severe damage which occurred to the instrumentation and structures in the 25 m array during the spills. Unfortunately, the IR gas sensors were not calibrated for HNO_3 mists.

The total mass spilled during Eagle 3 was 6090 kg N_2O_4. The vapor flux results from the 25 m row of gas sensors indicate that only 1170 kg of N_2O_4 and NO_2 vapors passed through this array in the first 10 min. This is only 20% of the amount spilled. The discrepancy is very likely largely due to the HNO_3 mist and whatever N_2O_4 remains in the ground. In addition, low-level soil out-gassing could continue for many hours and account for some of the material even though source strength falls off dramatically after about 350 sec.

The NO_2 vertical concentration contours, calculated from the gas sensor array at 785 m downwind for the Eagle 3 spill are shown in Fig. 8. The contours were calculated assuming a linear variation of the NO_2 concentration data between sensors. Taking into account the formation of HNO_3 mist, the source rate can be estimated to be about 410 kg/min and 344 kg/min for Eagle 3 and 6 respectively. The details of these estimates are contained in McRae, March 1985.

PRELIMINARY NH_3 RESULTS

The NH_3 data have just recently been reduced to final form but at the time this manuscript was written had not been publicly released. Consequently, the results presented here should be considered preliminary.

The Desert Tortoise 4 test was the largest of the NH_3 series. The NH_3 was released as a horizontal jet, about 1 m above ground level, pointing downwind. The jet expanded rapidly, due to the flashing of liquid into vapor and aerosol, and was extremely turbulent. Very little liquid NH_3 pooled on the ground during the shorter tests; however, a noticeable pool was left at the end of the Desert Tortoise 4 test which lasted for over six minutes. This pool represented only a small percentage of the total liquid spilled. Thus, most of the released NH_3 was immediately airborne either as cold vapor or aerosol. The cloud demonstrated noticeable dense gas effects, such as gravity driven slumping and spreading, as soon as the strong jetting and turbulence effects associated with the release were overcome. These source related effects were still present in the mass-flux arc of sensors at 100 m downwind but appeared from photographs to be considerably damped by the time the cloud reached twice this distance downwind. The vapor and aerosol plume, measured at the 100 m arc was considerably wider for test 4 than for the other tests. This indicates that the effects of gravity slumping and increased atmospheric stability were already important at the 100 m arc even in the presence of strong jetting. Figure 9 shows an upwind view of the cloud passing through the first row of sensors, and Fig. 10 shows a side view of the cloud from the release point to a point approximately 300 m downwind. Gas concentration contours in the vertical plane at the 800 m row of stations are shown in Fig. 11.

The maximum gas concentration as a function of downwind distance is given in Table IV for Desert Tortoise spill tests 2 through 4. The measured maximum gas concentrations from the Desert Tortoise 4 test are plotted in Fig. 12 along with predictions by the modified transient Gaussian plume model (Leitner, 1983) and the FEM3 model (Chan, 1983).

TABLE IV. PRELIMINARY RESULTS FROM DESERT TORTOISE SERIES NH_3 SPILLS. MAXIMUM GAS CONCENTRATION VERSUS DOWNWIND DISTANCE

	Gas Concentration at Downwind Distance			
Test	100 m	800 m	1450 m	2800 m
1	5.8%	1.1%	-	-
2	9.0%	1.8%	> 0.5%	-
3	9.0%	1.6%	-	0.2%
4	6.5%	2.1%	-	0.5%

COMPARISON WITH MODEL PREDICTIONS

<u>N_2O_4 Results Compared to Several Simple Models</u>. The primary purpose of the Eagle test series was to determine the importance of the heavy gas dispersion aspects of N_2O_4 vapors. Heavy gas clouds are lower and wider than those from a trace of neutral gas; their flow behavior is often dominated by gravity and they can exclude or displace the normal wind flow as would a solid object. This can sometimes result in a larger hazardous corridor downwind and in a more persistent, long lasting hazardous condition. The NO_2 concentration results from the Eagle 3 and Eagle 6 tests have been compared with the predictions of the Ocean Breeze/Dry Gulch (OB/DG) model (Haugen, 1963), Pasquill-Hanna Gaussian Plume model (Hanna, 1982), Shell dispersion model (Fleischer, 1980), and the CHARM model (Radian Corp., 1983).

A summary of these comparisons is given in Table V. The model predictions are compared to the peak measured concentration at 785m, and the cloud cross-section width (σ_y) and height (σ_z) determined from a best-fit Gaussian equivalent concentration distribution. Also included in Table V are the peak concentrations calculated by using the Gaussian cloud cross section and assuming conservation of the source strength mass flux. These larger peak concentration estimates are reasonable attempts to account for the unmeasured NO and HNO_3 gases known to be in the cloud, plus the uncertainty of obtaining the peak cloud concentration due to large-scale plume meander.

The comparison results indicate that all of the models examined substantially underpredict the measured peak NO_2 concentrations at 785 m. If we consider only the measured NO_2 results, the magnitude of the underpredictions range from a factor of about 4 for OB/DG to a factor of 2 for the CHARM model. If, however, the Gaussian equivalent/mass conservation estimates are used for the Eagle 3 and Eagle 6 tests (2275 and 575 ppm, respectively) then all of the models underpredict the results by factors ranging from 5 to 14. The predicted cloud cross-section dimensions, particularly the height, are substantially larger than measured. Thus, the simple models predict more mixing than is observed to occur, primarily as a result of using trace-gas plume-spread parameters which are averaged over long time periods and are independent of source strength and density.

TABLE V. Comparison Summary of the Eagle Test Results and Dispersion Model Predictions

	Peak Concentration (ppm)	σ_y (m)	σ_z (m)
EAGLE 3			
Test results			
Recorded	> 500		
Calculated+	2275	35	3.8
OB/DG	165	N/A	N/A
Gaussian Plume	163	60.5	31.9
Shell Dispersion	199	56.0	27.0
CHARM 220 60.5	23.6		
EAGLE 6			
Test results			
Recorded 315			
Calculated+	575	35	7.6
OB/DG	73	N/A	N/A
Gaussian Plume	89	60.5	31.9
Shell Dispersion	112	56.0	27.0
CHARM 127 58.7	23.2		

+Calculated from source strength using $Cp = \dot{m}_s/\pi\rho_v\sigma_y\sigma_z u$.

NH_3 Results Compared to the Modified Gaussian Plume and FEM3. The primary purpose of the NH_3 experiments was to measure the effect of aerosols on the dispersion of the NH_3 vapor. A three-dimensional hydrodynamic computer code (Kansa et al., 1983; Chan, 1983) has been used successfully to predict Liquefied Natural Gas dispersion and has recently been modified to include aerosol effects for high concentrations close to the spill point. For low concentrations, long distances downwind, the Gaussian model was believed to be adequate.

A modified transient Gaussian plume model was created to account for a finite duration release and various other problems found with Gaussian models (Leitner, Miller, Shinn, 1983; Koopman et al., 1984). The comparison of data from Desert Tortoise 4 and the modified transient Gaussian plume model is shown in Fig. 12. Clearly, the Gaussian calculation is inadequate. The data indicate that dense gas and aerosol effects exist well beyond the region near the spill point, to distances of at least 3 km downwind.

Since the calculation of dense gas/aerosol effects appears to be necessary for NH_3 spill predictions, a simple aerosol fog model was created for FEM3. The high-pressure release of NH_3 can result in as much as 83% of the material released forming a suspension of very fine droplets. The standard approach for treating a two-phase aerosol fog in a hydrodynamics code would be to add the additional partial differential equations (PDEs) for mass, momentum, and energy conservation of the liquid phase to the existing FEM3 model. In three dimensions, such an approach is computationally very expensive. Other approaches for dealing with the two-phase problem are reported in the PNL report (1981) and Kaiser and Walker, (1978).

The approach taken by Kansa et al. (1983) was to capture the essential behavior of a negatively buoyant two-phase vapor-droplet fog while using a conceptually simple model of the physics. Special physical features of the two-phase fog are the high average density of the fog, due to the liquid droplets, and the considerable amount of heat that must be added to the cloud in order to evaporate the droplets. The PDEs were solved for mass, momentum, energy, and species by assuming the aerosol fog to be a special type of vapor.

The behavior of the two-phase fog as it approaches a pure vapor cloud is modeled by means of a continuous temperature-dependent molecular weight and heat capacity. The simplifying assumptions are that the transition from liquid to vapor phase is accomplished over a temperature range, ΔT, over which the cloud is continuously transformed from a mixture of droplets (liquid phase) and vapor to pure vapor. The other assumption is that the fog behaves, over small pressure ranges, as an ideal gas. The approximations used are justified by focusing solely upon the governing physics of the dense gas dispersion, and ignoring the details of the suspension of NH_3 droplets. This is generally acceptable since interest in the details of cloud composition is focused downwind at lower concentrations.

A FEM3 calculation of the Desert Tortoise 4 60-m^3 ammonia spill, using the simple aerosol model, is shown in Fig. 12. The spill rate was 9.5 m^3/min, wind speed was 4.5 m/s and atmospheric stability was category E, as listed in Table II. The calculation predicts concentrations which are high by about a factor of two over the entire range of downwind distances. It is currently believed that this discrepancy is due primarily to the assumption that the maximum possible amount of aerosol (83%) is created when the ammonia is released. The actual amount of aerosol produced is not yet known but should be available once the aerosol data has been analyzed. It is likely to be less than 83% and may account for some of the discrepancy in concentration. It is also possible that the gaseous source strength was actually only about half of the release rate calculated due to interactions with water vapor and impact on the ground both at the spill point and downwind. This will be clarified in an upcoming report (Goldwire, in preparation). The measured cloud width and height are similar to that predicted by the model.

Another important aspect of the comparison between calculation and data is that the falloff of concentration with distance (slope) is similar. Thus, the model calculation is also predicting the importance of the dense gas and aerosol effects at long distances downwind observed in the data. How far these effects persist downwind is still unknown and should be the goal of some future experimental and modeling work. The data show no hint of trace gas behavior even at 2800 m downwind, yet, there is reason to believe that concentration will eventually exhibit trace gas behavior, falling off with distance with the same slope as that of the Gaussian model.

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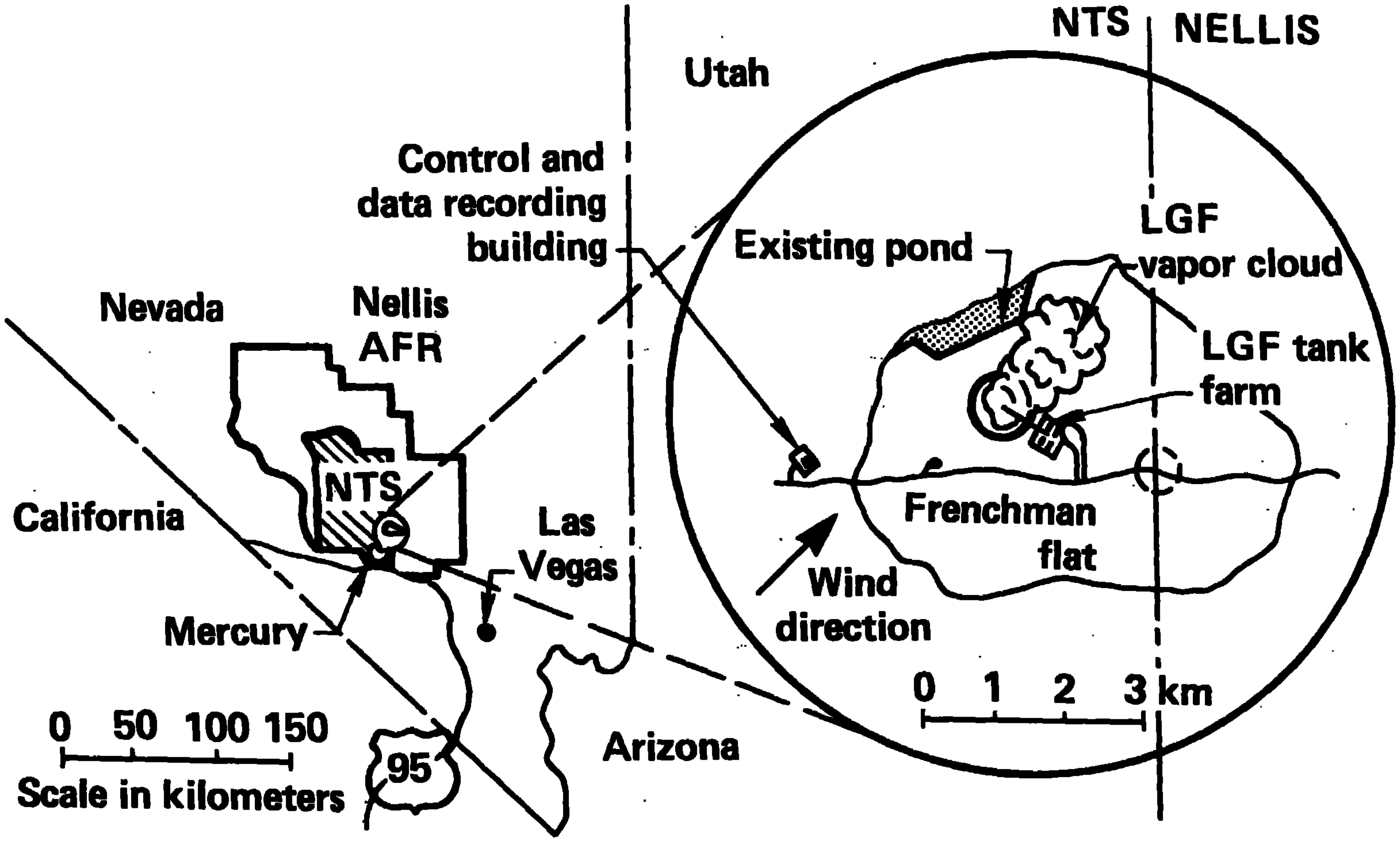

Figure 1. The new DOE LGF Spill Test Facility is being built on Frenchman Flat at the Nevada Test Site.

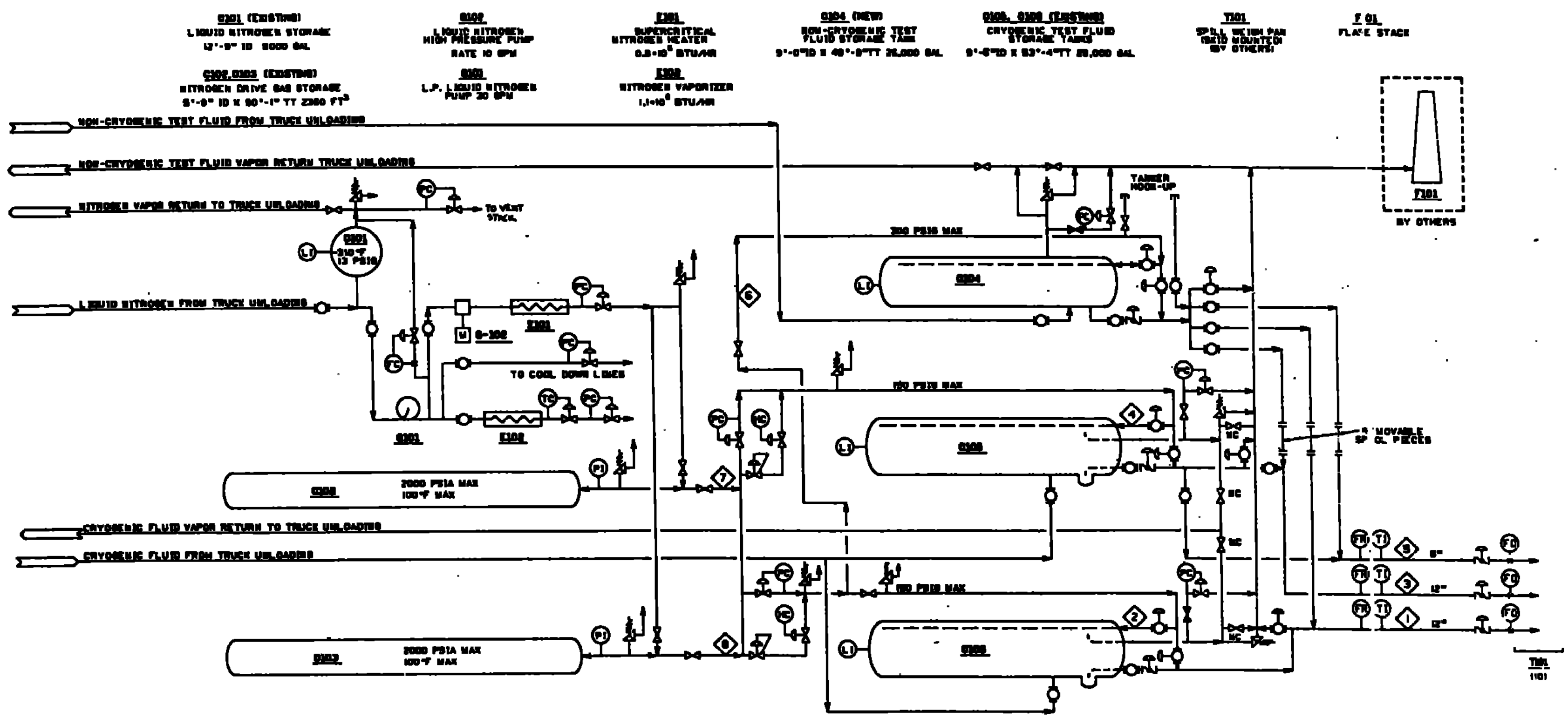

Figure 2. Process flow diagram for the LGF Spill Test Facility.

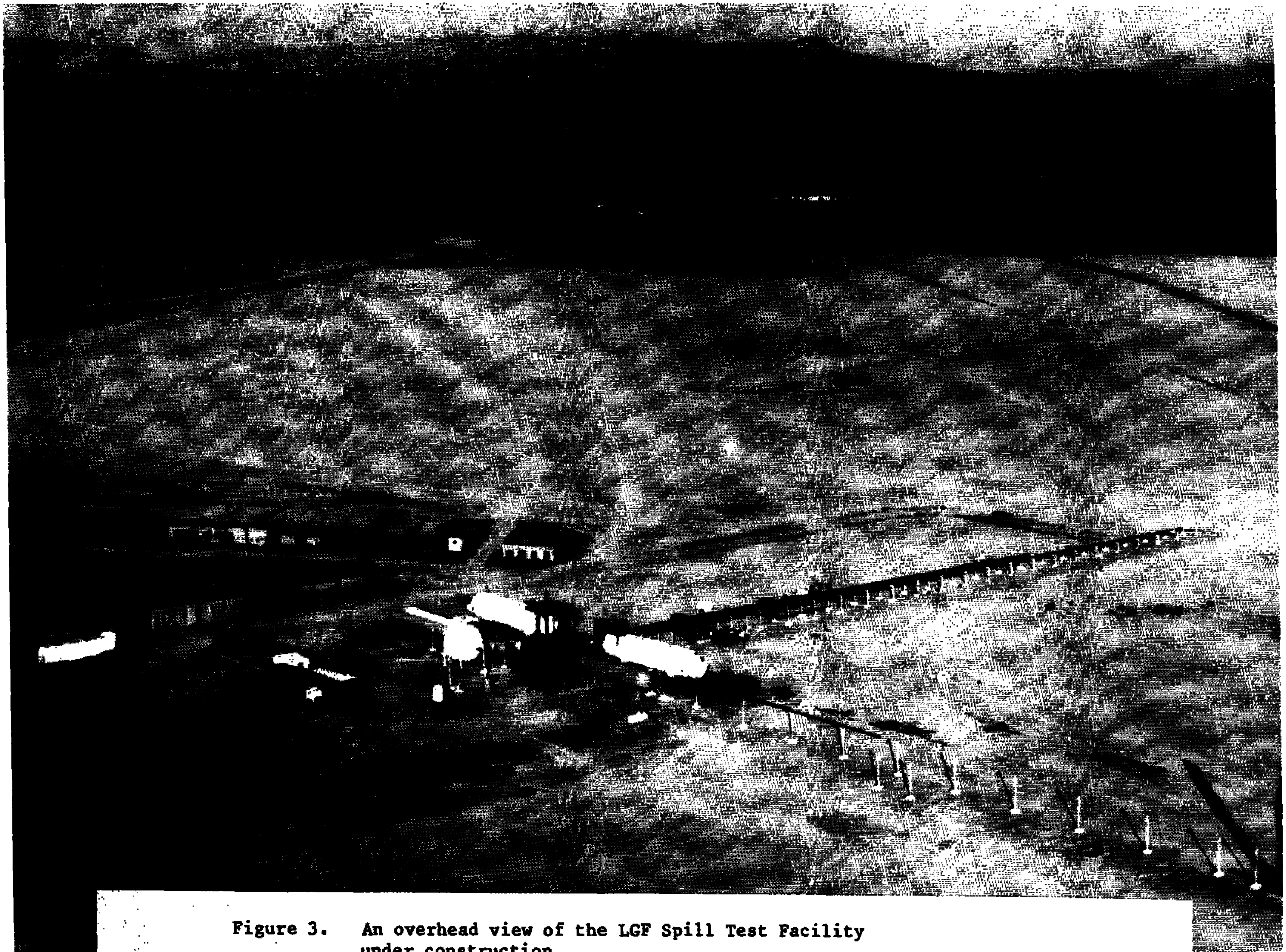

Figure 3. An overhead view of the LGF Spill Test Facility under construction

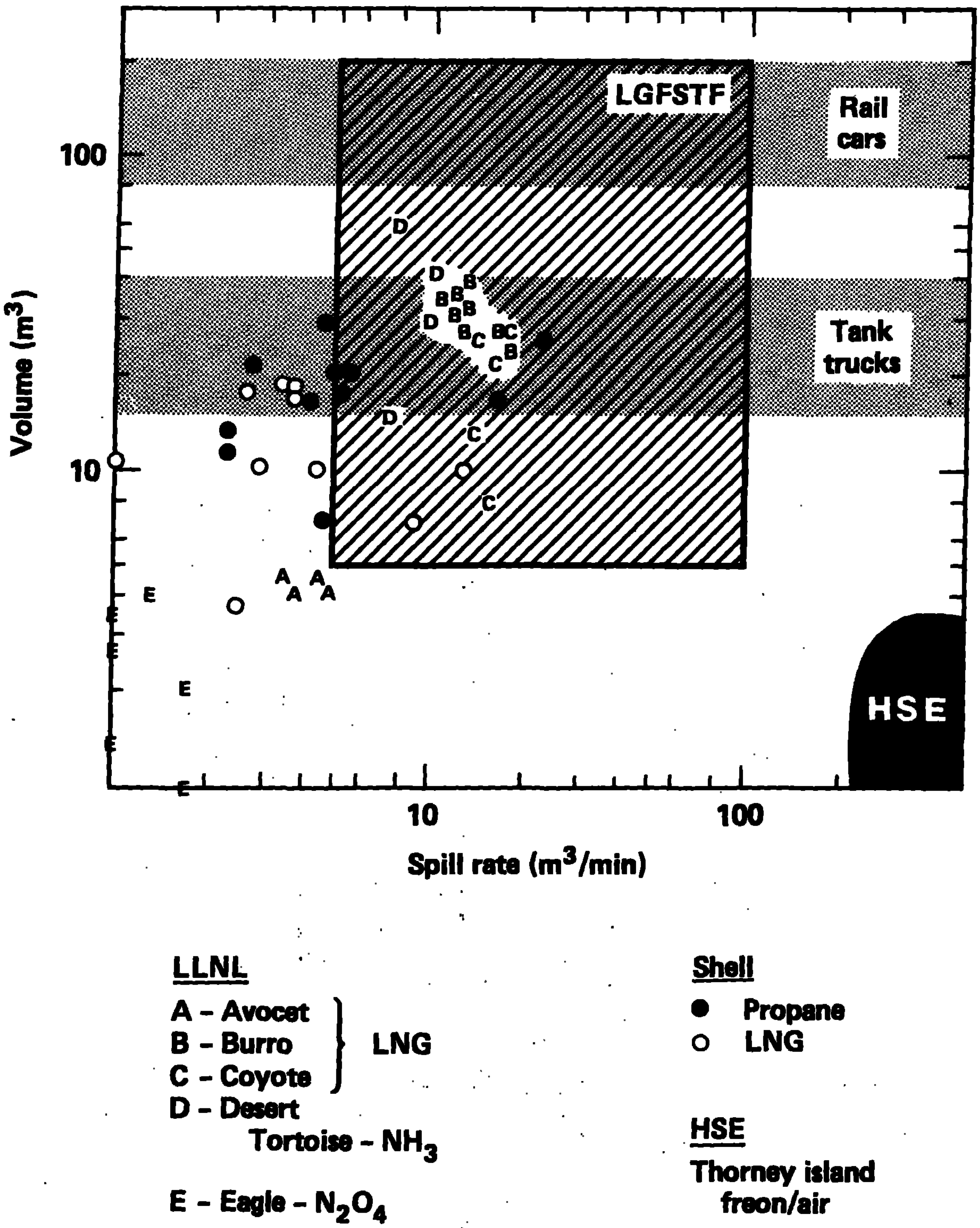

Figure 4. The new DOE LGF Spill Test Facility will allow experiments in a critical regime.

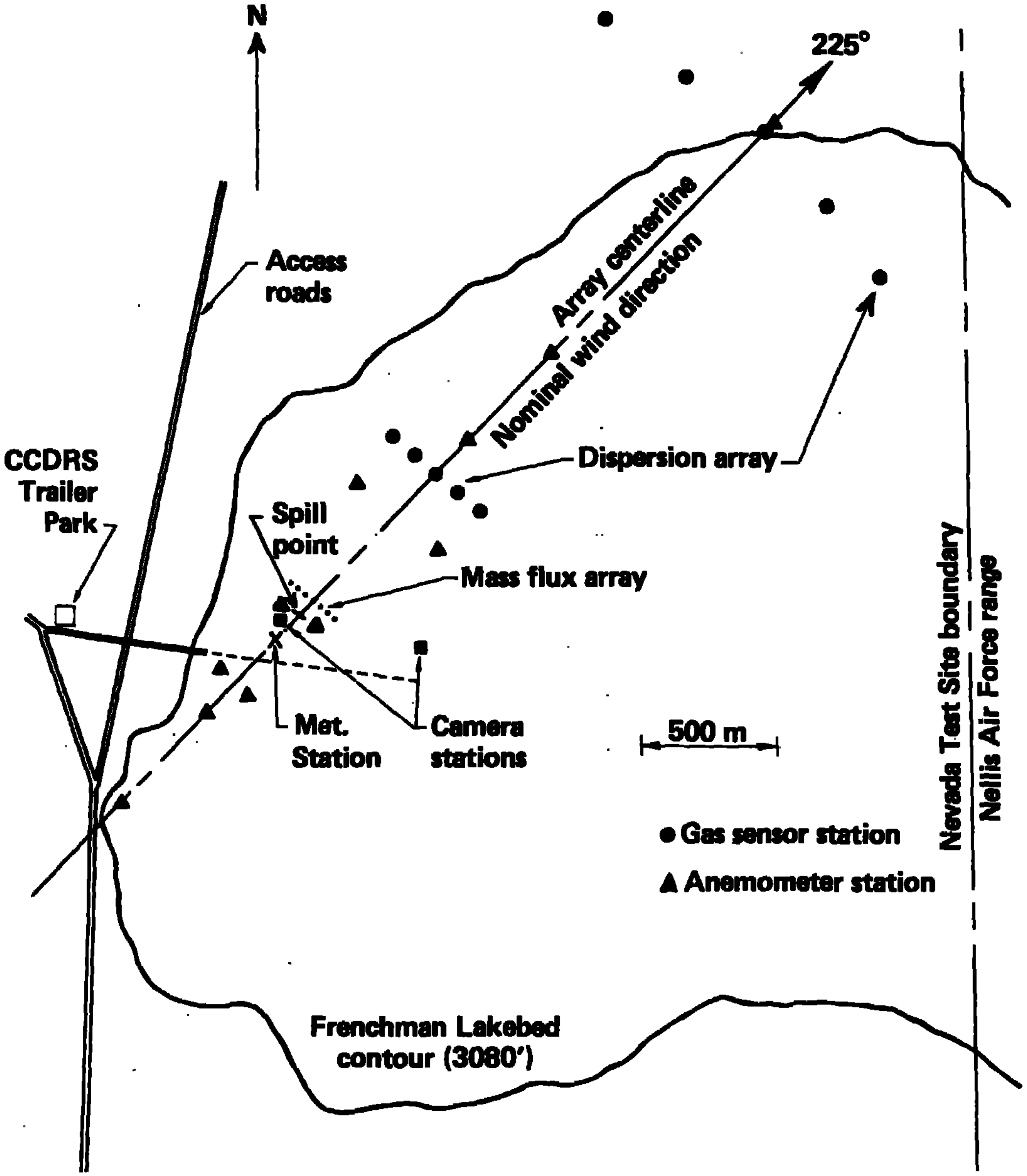

Figure 5. Diagnostic instrument array for Desert Tortoise and Eagle series experiments.

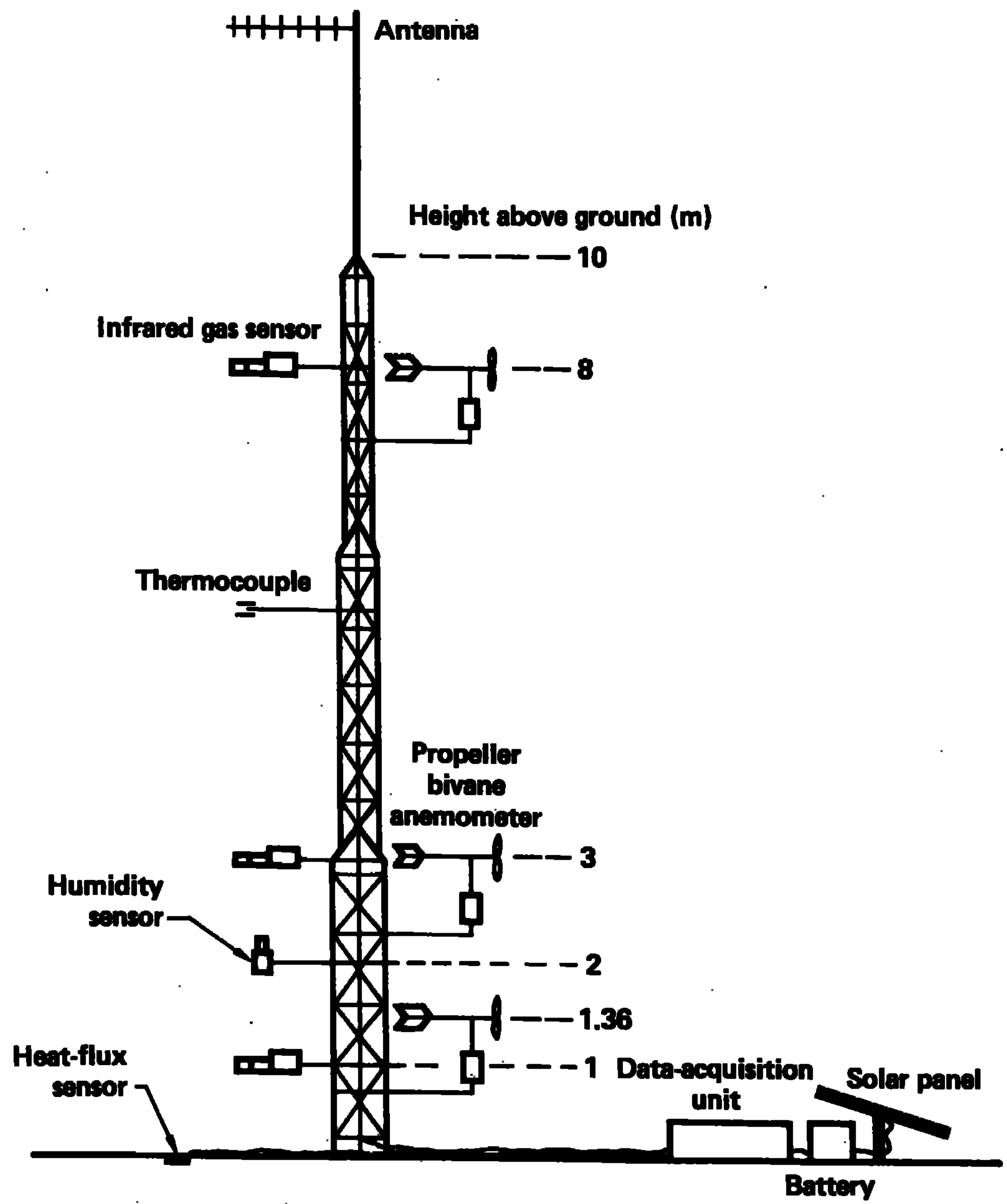

Figure 6. A typical gas sensor station showing many of the instruments used for measurement of the dispersing gas cloud.

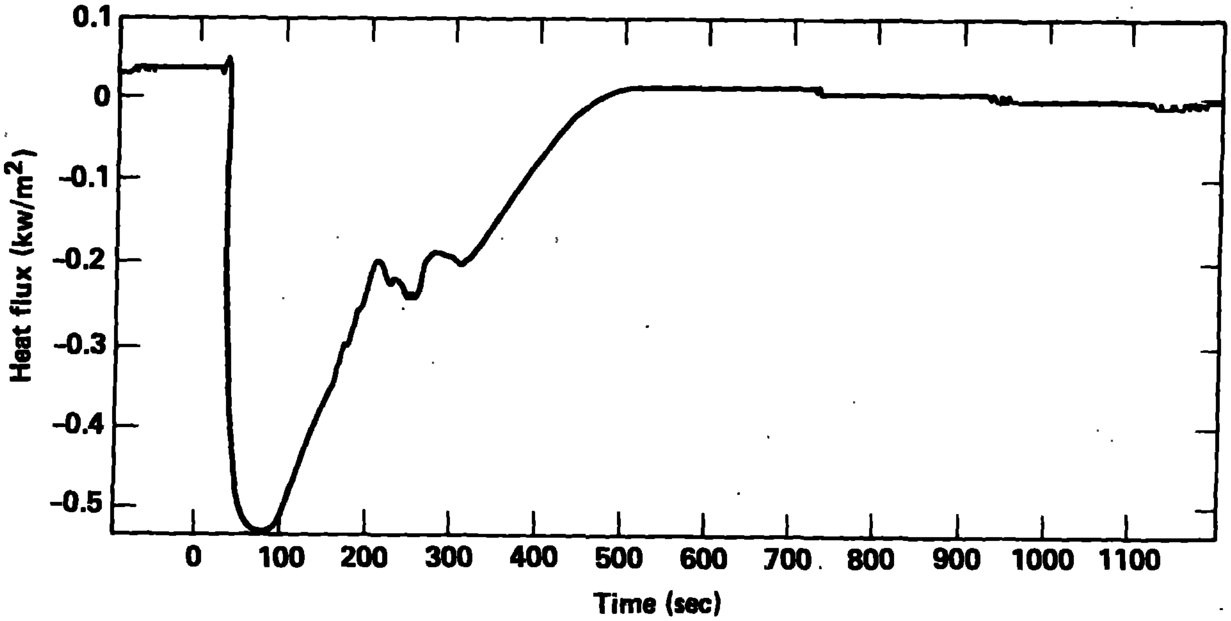

Figure 7. Eagle 3 spill area heat flux data.

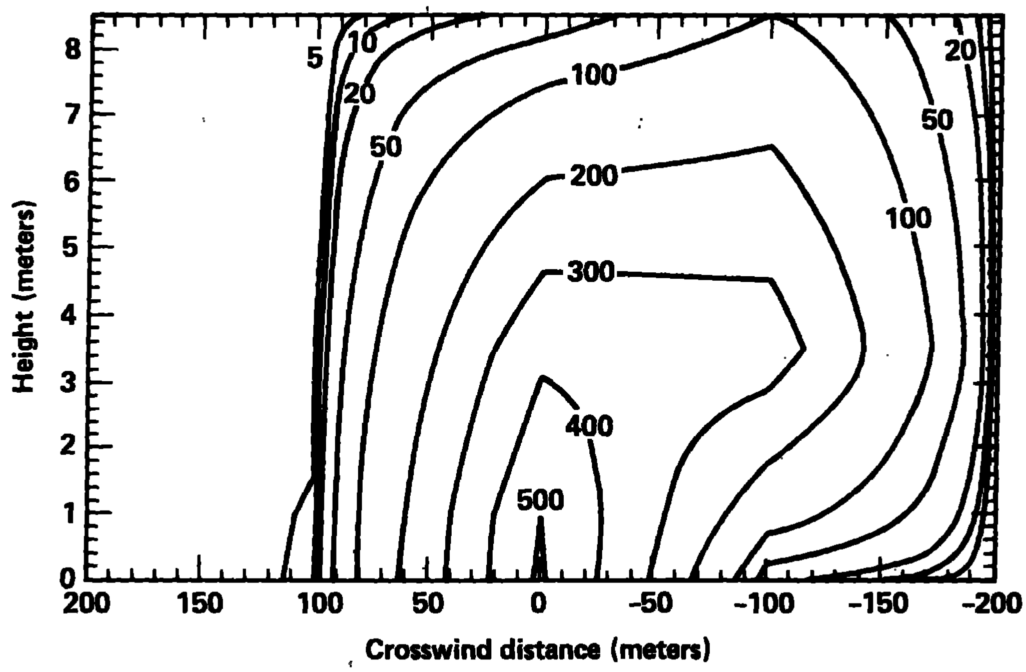

Figure 8. Eagle 3 crosswind concentration contours at 785 m.

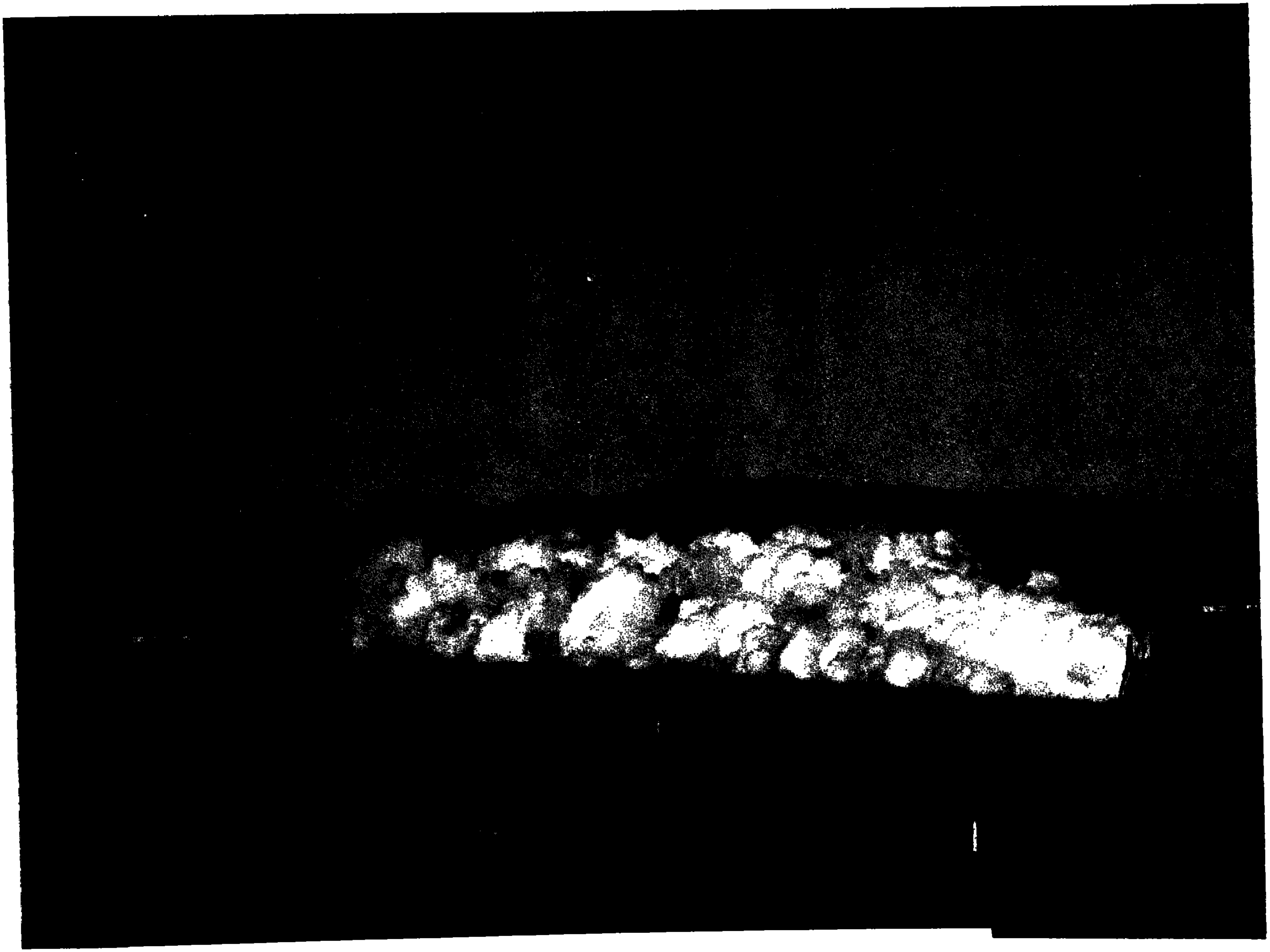

Figure 9. Desert Tortoise 4 spill seen from upwind camera.

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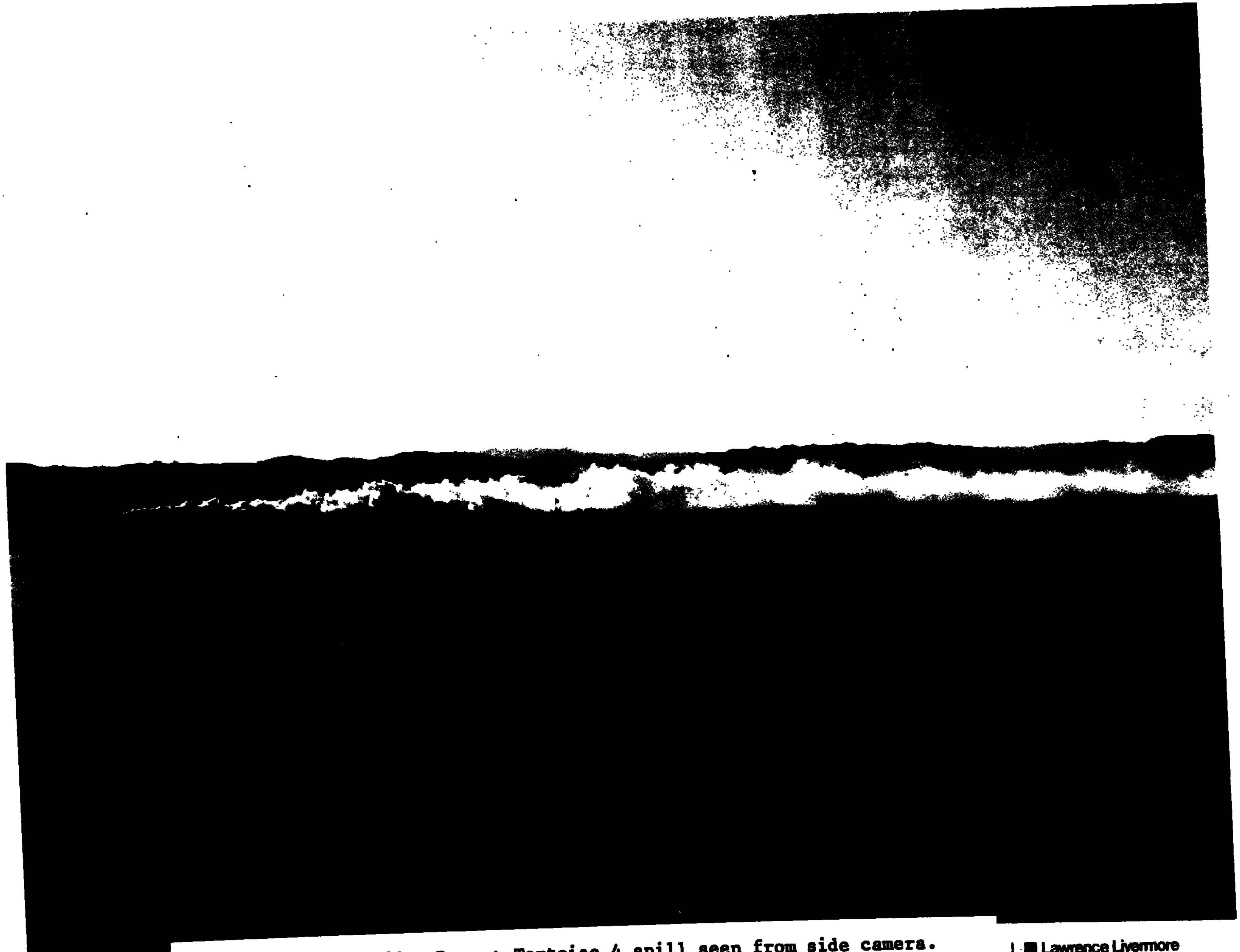

Figure 10. Desert Tortoise 4 spill seen from side camera.

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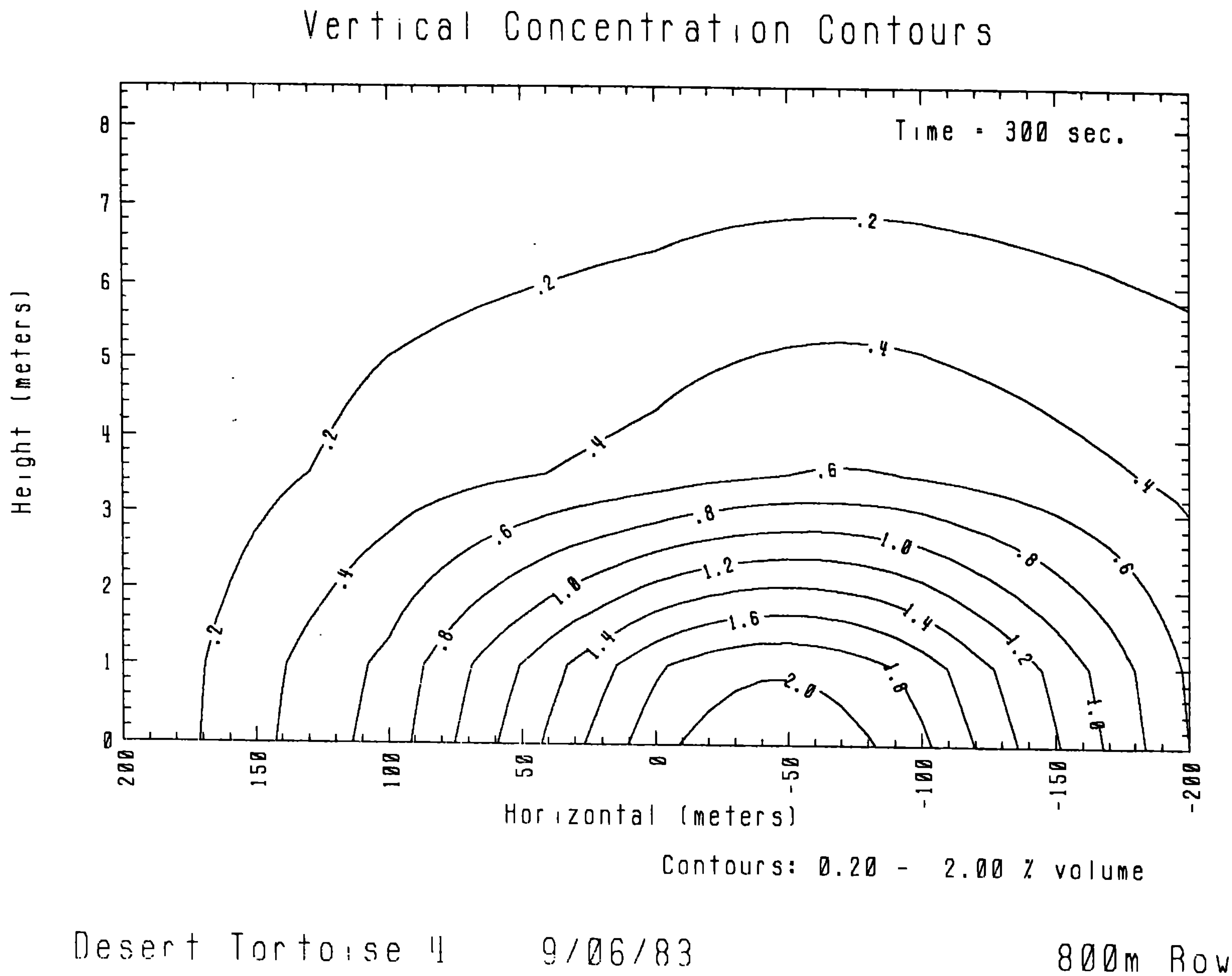

Figure 11. Gas concentration in the vertical plane at the 800 m row.

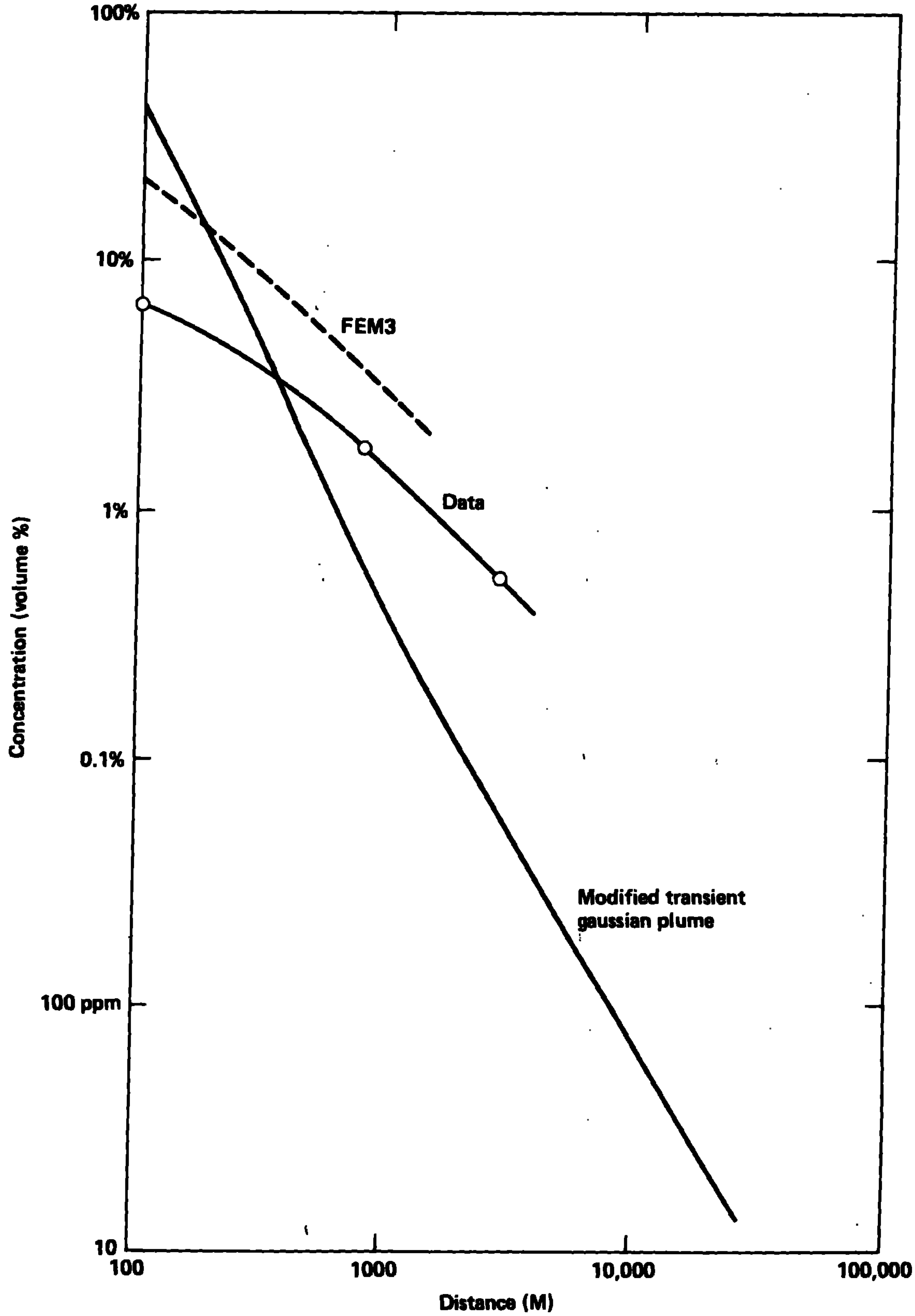

Figure 12. Model data comparison for Desert Tortoise 4 60 m^3 ammonia spill.